Homogeneous Dislocation Nucleation and Anomalous Hardening in RDX

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The plastic deformation of crystalline solids is usually mediated by the motion of dislocations. Dislocations glide on crystallographic planes and the displacement they produce is known as the Burgers vector. Under typical loading conditions, dislocations nucleate and multiply heterogeneously by the formation and/or activation of dislocation sources. However, under shock loading, dislocation loops may nucleate homogeneously [1]. We recently discovered homogeneous nucleation of dislocations in the energetic molecular crystal cyclotrimethylene trinitramine (RDX) using non-equilibrium molecular dynamics (NEMD) simulations [2]. This unexpected deformation mechanism allowed us to quantitatively explain some puzzling experimental results.

Flyer-plate-driven shock waves with shock pressure P = 1.25 GPa in (111)-oriented RDX single crystals revealed an elastic-plastic response that was expected based on the orientation of the shock with respect to the known slip systems [2]. However, at P = 2.25 GPa we saw a single-wave, overdriven response [3] that suggested an abrupt change in the underlying mechanisms of plastic deformation with increasing pressure [2]. Interface velocity (VISAR) traces for shocks at P = 1.25 and 2.25 GPa are presented in Fig. 1 (a) and (b), respectively.

Multi-million atom NEMD simulations of the propagation of planar shock waves normal to (111) were performed using an accurate and transferable potential for RDX. Crystal defects were not nucleated at P = 1.4 GPa. However, for $P \geq 1.8$ GPa, partial dislocation loops enclosing a stacking fault were nucleated homogeneously on (001). The Burgers vector of the partials was identified as $\mathbf{b} = 0.16[010]$ by calculating the [010] cross-section of the (001) γ-surface [2,4]. The partial dislocations are highly mobile and rapidly generate stacking faults throughout the shocked material. Furthermore, analysis of the conformation of RDX molecules at the stacking fault showed that it is rendered metastable by a change in the orientation of the nitro groups with respect to mean plane of the six-member ring. In Fig. 2, we show only those molecules that have changed conformation, and hence the stacking faults, for a NEMD simulation at 2.2 GPa.

The stacking faults intersect the slip planes of the perfect dislocations that are responsible for the well-defined plastic wave seen experimentally at P = 1.25 GPa. Thus, above the threshold shock pressure for homogeneous nucleation, $1.4 < P_{th} \leq 1.8$ GPa, the material becomes plastically very hard because the stacking faults are obstacles to the glide of perfect dislocations. For this reason, above P_{th}, an overdriven rather than two-wave structure is found experimentally.

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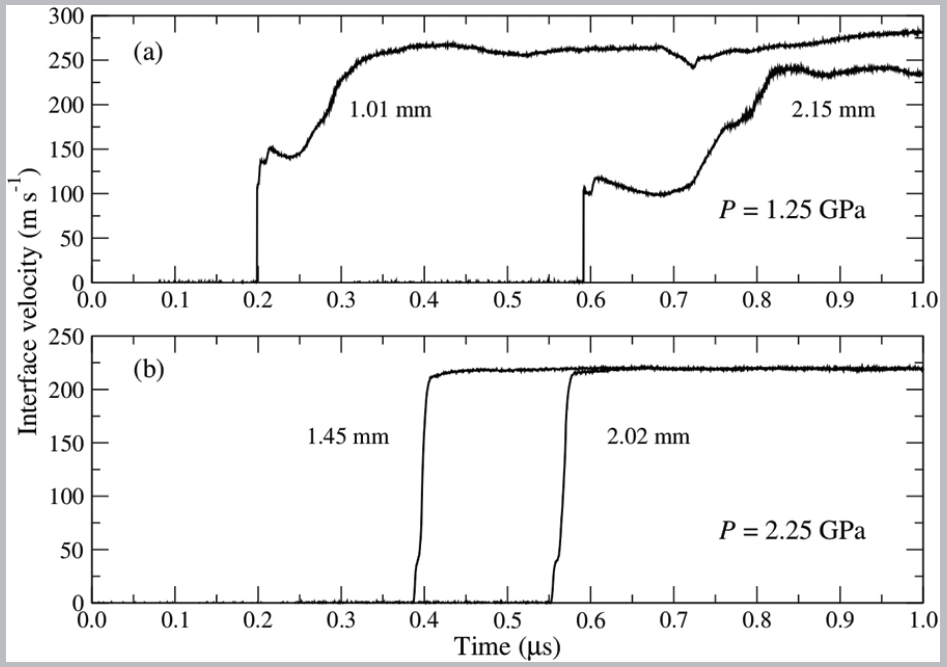

Fig. 1. VISAR interface velocity traces for flyer-plate-driven shock waves in (111)-oriented RDX single crystals. (a) P = 1.25 GPa, (b) P = 2.25 GPa.

Fig. 2. NEMD simulation cell measuring 138.8 x 21.3 x 19.3 nm at the time of maximum compression during shock loading at P = 2.2 GPa. The shock front propagated from left to right. The centers of mass of those molecules that changed conformation are shown. The stacking faults on (001) are visible as ribbons in this projection.